

**Table 1. Exemplary Nanotag Elements**

| <b>Molecules</b>                                     | <b>Vender</b>   | <i>MW</i><br><i>g/mol</i> | <b>Distinguishable Features</b>             |
|--|-----------------|---------------------------|---|
| <b>Fullerenes</b>                                    |                 |                           |   |
| C60  | BuckyUSA        | 720.6                     | size, shape, low density                    |
| C70  | BuckyUSA        | 840.7                     | size, shape, low density                    |
| C84  | BuckyUSA        | 1008.9                    | size, shape, low density                    |
| <b>Metal Center Fullerenes</b>                       |                 |                           |   |
| C60La  | BuckyUSA        | 859.5                     | size, shape, high electron density & charge |
| C84La  | BuckyUSA        | 1147.8                    | size, shape, high electron density & charge |
| C60Er  | BuckyUSA        | 887.5                     | size, shape, high electron density & charge |
| C84Er  | BuckyUSA        | 1176.8                    | size, shape, high electron density & charge |
| <b>Fullerene Oxides</b>                              |                 |                           |   |
| C60-O  | BuckyUSA        | 736                       | size, shape, low density                    |
| C70-O  | BuckyUSA        | 856                       | size, shape, low density                    |
| <b>Bifunctional Fullerenes</b>                       |                 |                           |   |
| O-C60-O  | BuckyUSA        | 752                       | size, shape, low density                    |
| O-C70-O  | BuckyUSA        | 872                       | size, shape, low density                    |
| <b>P.O.S.S. Polyhedral oligomeric silsesquioxane</b> | Hybrid Plastics | 800-1600                  | 800-1600                                    |
| Octakis pentacyclo octasiloxane hydrate              | Aldrich         | 1137                      | Size, shape, charge (-)                     |
| OctaAmmonium POSS                                    | Hybrid Plastics |                           | Size, shape, charge (+)                     |
| OctaIsobutyl POSS                                    | Hybrid Plastics |                           | size, shape                                 |
| OctaMethyl POSS                                      | Hybrid Plastics |                           | size, shape                                 |
| Octa TmA POSS  | Hybrid Plastics |                           | size, shape, density                        |

**Table 1 (continued)**

| <b>Organometallics</b>  |                                    |        |  |
|---|------------------------------------|--------|--|
| Metal Centers include:Cr, Fe, Al, B, Co, Ni, Zr, Cu, Mg, Zn and Ru. Organic moieties include any functionalizable structure including, sepulcrates, bipyridines, porphrines, corrins, EDTA, biphenyl, benzene, phthalocyanine, hematoporphyrin, heme, naphthalocyanine, phthalocyanine, Cyclopentadiene, Indene, Fluorene, Benzoindene, 4-Fluorophenyl, 4-Methoxypheny, Tris(4-chlorophenyl) and others | Aldrich, Acros, Boulder Scientific |        | Metal centers have different size of outer orbital, density, charge distribution, and redox states. The organic moieties impart size, shape and density characteristics. |
| Cu II trifluoroacetyl acetate   | Aldrich                            |        |  |
| Cu II phthalocyanine  | Aldrich                            |        |  |
| Co II phthalocyanine  | Aldrich                            |        |  |
| Fe II phthalocyanine  | Aldrich                            |        |  |
| Zn II phthalocyanine  | Aldrich                            |        |  |
| Ni II phthalocyanine  | Aldrich                            |        |  |
| Mg II phthalocyanine  | Aldrich                            |        |  |
| Co II 2-3 naphthalocyanine  | Aldrich                            |        |  |
| 1,1'-Ferrocenedicarboxylic acid   | Aldrich                            | 274.06 |  |
| Co III sepulcrate trichloride   | Aldrich                            |        |  |
| Cu II 2-pyrazinecarboxylate   | Aldrich                            |        |  |
| Nano-crystal particle (Ag), NHS esters  | Nanoprobes                         |        |  |

**TABLE 2. Potential Subunits for Backbone Mediated Synthesis**

| <b>Candidate</b>                     | <b>Monofunctionalized</b> | <b>Attachment to subunit</b>         |
|--------------------------------------|---------------------------|--------------------------------------|
| C60                                  | C60COOH                   | Lysine                               |
| C70                                  | C70COOH                   | Lysine                               |
| La Buckey                            | LA Bucky COOH             | Lysine                               |
| C60                                  | C60COOH                   | Ethyl amino Thymidine                |
| C70                                  | C70COOH                   | Ethyl amino Thymidine                |
| La Buckey                            | LA Bucky COOH             | Ethyl amino Thymidine                |
| (NH <sub>2</sub> ) <sub>8</sub> POSS | NA                        | Glutamic or aspartic acid            |
| Metal Phalocyanonine                 | COOH                      | Lysine or NH <sub>2</sub> -Thymidine |
| <b>Metal Phalocyanonine</b>          | NH <sub>2</sub>           | Glutamic or aspartic acid            |

**Table 3. Exemplary Subunits for Polymer Decoration**

| Tag Element                          | Mono-functionalized | Attachment to polymer subunit | Polymer sequence                                      |
|--------------------------------------|---------------------|-------------------------------|---|
| C60                                  | C60COOH             | Lysine                        | NH <sub>2</sub> -(Gly-Gly-Gly-Lys) <sub>8</sub> -COOH |
| C60                                  | C60COOH             | Lysine                        | NH <sub>2</sub> -(A-A-A-A-A-A-K) <sub>7</sub> -COOH   |
| C70                                  | C70COOH             | Lysine                        | NH <sub>2</sub> -(Gly-Gly-Gly-Lys) <sub>8</sub> -COOH |
| C70                                  | C70COOH             | Lysine                        | NH <sub>2</sub> -(A-A-A-A-A-A-K) <sub>7</sub> -COOH   |
| La Buckey                            | LA Bucky COOH       | Lysine                        | NH <sub>2</sub> -(Gly-Gly-Gly-Lys) <sub>8</sub> -COOH |
| La Buckey                            | LA Bucky COOH       | Lysine                        | NH <sub>2</sub> -(A-A-A-A-A-A-K) <sub>7</sub> -COOH   |
| C60                                  | C60COOH             | Ethyl amino Thymidine (X)     | 5'-(T-X)10-3'   |
| C60                                  | C60COOH             | Ethyl amino Thymidine (X)     | 5'-(X-Q) where Q is 12 atom spacer                    |
| C70                                  | C70COOH             | Ethyl amino Thymidine (X)     | 5'-(T-X)10-3'   |
| C70                                  | C70COOH             | Ethyl amino Thymidine (X)     | 5'-(X-Q) where Q is 12 atom spacer                    |
| La Buckey                            | LA Bucky COOH       | Ethyl amino Thymidine (X)     | 5'-(T-X)10-3'   |
| La Buckey                            | LA Bucky COOH       | Ethyl amino Thymidine (X)     | 5'-(X-Q) where Q is 12 atom spacer                    |
| (NH <sub>2</sub> ) <sub>8</sub> POSS | NA                  | Glutamic or aspartic acid     | NH <sub>2</sub> -(Gly-Gly-Gly-Glu) <sub>8</sub> -COOH |
| (NH <sub>2</sub> ) <sub>8</sub> POSS | NA                  | Glutamic or aspartic acid     | NH <sub>2</sub> -(A-A-A-A-A-E) <sub>7</sub> -COOH     |
| (NH <sub>2</sub> ) <sub>8</sub> POSS | NA                  | T carboxylate analog (Y)      | 5'-(T-Y)10-3'   |
| Metal Phalocyanine                   | COOH                | Lysine                        | NH <sub>2</sub> -(A-A-A-A-A-A-K) <sub>7</sub> -COOH   |
| Metal Phalocyanine                   | COOH                | Lysine                        | NH <sub>2</sub> -(Gly-Gly-Gly-Lys) <sub>8</sub> -COOH |

**Table 4. Exemplary Subunits for Direct Polymer Imaging**

| <b>Subunit</b>         | <b>Polymer</b>   |
|------------------------|--|
| Lysine (K)             | (A <sub>6</sub> -K) <sub>8</sub> or (AAKAAAK) <sub>4</sub> or KKKKKKKK |
| Glutamic acid (E)      | (A <sub>6</sub> -E) <sub>8</sub> or (AAEAAAE) <sub>4</sub> or EEEEEEE  |
| E and K                | (AAKAAAE) <sub>4</sub>   |
| Br-T (Br)              | T-Br-T-Br-TTT-Br-TTT-Br-Br-T   |
| NH <sub>2</sub> -T (N) | T-N-T-N-TTT-N-TTT-N-N-T  |
| Br and N               | T-Br-T-N-T-Br-Br-TTT-N-N-Br-T  |
| Phosphate and spacers  | TTT-3-9-3-3-9-9-3-9  |